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Single Crystal Gradient Plasticity – Part III
Outline

Motivation

Dislocation continuum theories – overview

The concept of lifted curves

Modelling of pile-ups

Numerical results

Conclusion and Outlook
Literature

- **Fundamental dislocation theory**
  e.g. Taylor (1934); Orowan (1935); Schmid and Boas (1935); Hall (1951); Petch (1953)

- **Kinematics and crystallographic aspects of GNDs**
  Nye (1953); Bilby, Bullough and Smith (1955); Kröner (1958); Mura (1963); Arsenlis and Parks (1999)

- **Thermodynamic gradient theories**
  e.g. Fleck et al. (1994); Steinmann (1996); Menzel and Steinmann (2001); Liebe and Steinmann (2001); Reese and Svendsen (2003); Berdichevski (2006); Ekh et al. (2007); Gurtin, Anand and Lele (2007); Fleck and Willis (2009); Bargmann et al. (2010); Miehe (2011)

- **Slip resistance dependent on GNDs and SSDs**
  e.g. Becker and Miehe (2004); Evers, Brekelmans and Geers (2004); Cheong, Busso and Arsenlis (2005)

- **Micromorphic approach**
  e.g. Forest (2009); Cordero et al. (2010); Aslan et al. (2011)

- **Continuum Dislocation Dynamics**
  e.g. Hochrainer (2006); Hochrainer, Zaiser and Gumbsch (2007); Hochrainer, Zaiser and Gumbsch (2010); Sandfeld, Hochrainer and Zaiser (2010); Sandfeld (2010)
Dislocation Microstructure

Spiral source  Cell structures at different deformation stages  Single dislocations

Important features of the microstructure
- Total line length/density
- Dislocation sources
- Dislocation motion/transport
- Lattice distorsion
Classical Continuum Dislocation Measures

Total line length per unit volume

\[ \rho = \frac{\Delta l_{\text{tot}}}{\Delta V} \]

Typical (local) evolution law:

\[ \partial_t \rho = f(\dot{\gamma}, \rho) \]

Transport neglected!

Nye’s dislocation density tensor

\[ \alpha = \text{curl} \left( H^p \right) \]

SSDs neglected!

\( H^p \): plastic displ. gradient
Smooth Dislocation Bundles

Mura (1963)

Dislocation density vector

\[ \kappa := \rho e_l \]

Effective 'Number' of penetration points

\[ N_{\text{eff}} = \int_A \kappa \cdot d\alpha, \]

Dislocation flux into \( A \)

\[ \dot{N}_{\text{eff}} = - \int_{\partial A} (\kappa \times \nu) \cdot e_T \, ds, \]

\[ \Rightarrow \partial_t \kappa = - \text{curl} (\kappa \times \nu) \]

Closed evolution equation

Holds if nearby dislocations are parallel!

How to treat non-parallel dislocations?
Concept of lifted dislocations

Hochrainer (2006); Hochrainer, Zaiser and Gumbsch (2007)

If curvature depends on position and orientation $k = k(x_1, x_2, \varphi, t)$:

Adjacent lifted dislocations are parallel!

Lift the dislocations according to their local orientation $\varphi$

Lifted parallel curves
Concept of lifted dislocations

Hochrainer (2006); Hochrainer, Zaiser and Gumbsch (2007)

Density vector of lifted dislocations

\[ \kappa^I = \rho^I e^I \]

\( \rho^I \): Density of lifted dislocations

\( e^I \): line direction

Velocity of the lifted dislocations

\[ V = \nu + a \vartheta e_3 \]

\( \nu \): real dislocation velocity

\( \vartheta \): angular velocity

Evolution equation (by analogy)

\[ \partial_t \kappa^I = -\text{curl} (\kappa^I \times V) \]

Planar projection of \( \kappa^I \)

Derivation of orientation dependent density \( \rho^\varphi (x_1, x_2, \varphi, t) = a \kappa^I \cdot e^I \)

Total dislocation density

\[ \rho(x_1, x_2, t) = \int_0^{2\pi} \rho^\varphi d\varphi \]
Continuum Dislocation Dynamics (CDD)

Evolution equation of lifted dislocation density vector

\[ \partial_t \kappa^{II} = - \text{curl} (\kappa^{II} \times \mathbf{V}) \]

\[ \kappa^{II} = \frac{\rho}{a} e_l + \rho \varphi k_e_3 \]

Equivalent: Evolution equations of density \( \rho^\varphi \) and curvature \( k \)

\[ \partial_t \rho^\varphi = - \text{div} (\rho^\varphi \mathbf{v}) - \partial_\varphi (\rho^\varphi \partial_\varphi) + \rho^\varphi k \nu \]

\[ \partial_t (\rho^\varphi k) = - \text{div} (\rho^\varphi k \nu - \rho^\varphi \partial_\varphi e_l) \]

Averaged/Simplified Theory (sCDD)

Averaged field variables

\[ \rho(x_1, x_2, t) = \int_{0}^{2\pi} \rho^\varphi d\varphi \]

\[ \bar{\rho}k(x_1, x_2, t) = \int_{0}^{2\pi} \rho^\varphi k d\varphi \]

\[ \kappa^\perp = \int_{0}^{2\pi} \rho^\varphi e_\nu d\varphi \]

Averaged evolution equations

\[ \partial_t \rho = - \text{div} (\kappa^\perp \nu) + \bar{\rho}k \nu \]

\[ \partial_t \bar{\rho}k = - \text{div} (\bar{\rho}k/\rho \nu \kappa^\perp + \rho/2 \nabla_\rho \nu) \]
Comparison of Dislocation Theories

**Local density evolution models**
- explicit annihilation terms
- parameter calibration required
- dislocation transport neglected

**Gradient plasticity / GND-based models**
- \( \alpha = \text{curl}(H^p) \)
- no information on SSDs

**Simplified Continuum Dislocation Dynamics (sCDD)**
- SSDs are naturally included
- here: explicit annihilation not included (yet)

**Phenomenological hardening approach required**
- \( \tau^C = \tau^C(\rho, ...) \)
- no parameter calibration for kinematics

**Computation of strain gradients / pile-ups**
- accounts explicitly for dislocation transport
- dislocation curvature information

**All dislocations are included**

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\( \partial_t \rho = \text{div}(\ldots) + \ldots \)
Coupling to Crystal Plasticity

**Single slip framework**
- Additive decomposition
- Plastic distortion
- Elastic strain
- Stress
- Resolved shear stress

**Coupling equations**
- Orowan equation
- Overstress modell
- Taylor hardening

**PDEs**
\[
\begin{align*}
\text{div} (\sigma) &= 0 \\
\partial_t \rho &= -\text{div} (\kappa^\perp \nu) + \rho k \nu \\
\partial_t \rho k &= -\text{div} \left( \frac{\rho k}{\rho} \nu \kappa^\perp + \rho/2 \nabla_p \nu \right)
\end{align*}
\]
Dislocation Starvation Simulation 1

Initial conditions

\[
\rho(x, t = 0) = \rho_0 = \text{const.}
\]

\[
k(x, t = 0) = k_0 \gg 1/L
\]

\[
\Rightarrow \rho k(x, t = 0) = \rho_0 k_0
\]

High viscosity required for stabilization

⇒ Homogeneous distribution of small loops

Videos 1, 2, 3

Force displacement curve
Dislocation Starvation Simulation 2

Initial conditions

\[ \rho(x, t = 0) : \text{concentrated at center} \]
\[ k(x, t = 0) = k_0 \gg 1/L \]

Videos 4, 5

⇒ Inhomogeneous distribution of small loops

Figure: Initial configuration

Figure: After loading
Numerical results

Initial conditions

\[ \rho(x, t = 0) = \rho_0 = \text{const.} \]

\[ k(x, t = 0) = k_0 \gg \frac{1}{L} \]

\[ \Rightarrow \rho k(x, t = 0) = \rho_0 k_0 \]

⇒ Homogeneous distribution of small loops

![Force displacement curve](image)
Conclusion

- There is a need for a continuum theory of dislocations to bridge the scales
- Concept of lifted curves → physically based continuum theory
- Takes into account
  - SSDs & GNDs
  - transport
  - curvature
- Fits into crystal plasticity framework
- Facilitates the simulation of effects like dislocation starvation
Thank you for your attention

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